



ADMET Group Leaderboard

[TDC.Caco2_Wang](#) Leaderboard

[TDC.Bioavailability_Ma](#) Leaderboard

[TDC.Lipophilicity_AstraZeneca](#) Leaderboard

[TDC.Solubility_AqSolDB](#) Leaderboard

[TDC.HIA_Hou](#) Leaderboard

[TDC.Pgp_Broccatelli](#) Leaderboard

[TDC.BBB_Martins](#) Leaderboard

[TDC.PPBR_AZ](#) Leaderboard

[TDC.VDss_Lombardo](#) Leaderboard

[TDC.CYP2C9_Veith](#) Leaderboard

[TDC.CYP2D6_Veith](#) Leaderboard

[TDC.CYP3A4_Veith](#) Leaderboard

[TDC.CYP2C9_Substrate_CarbonMangels](#) Leaderboard

[TDC.CYP2D6_Substrate_CarbonMangels](#) Leaderboard

[TDC.CYP3A4_Substrate_CarbonMangels](#) Leaderboard

[TDC.Half_Life_Obach](#) Leaderboard

[TDC.Clearance_Hepatocyte_AZ](#) Leaderboard

[TDC.Clearance_Microsome_AZ](#) Leaderboard

[TDC.LD50_Zhu](#) Leaderboard

[TDC.hERG](#) Leaderboard

[TDC.AMES](#) Leaderboard

[TDC.DILI](#) Leaderboard

References

[Submission Instructions](#)

[BenchmarkGroup Class Documentation](#)

[Leaderboard Guidelines](#)

[TDC.Lipophilicity_AstraZeneca](#) Leaderboard

Dataset Summary

Dataset	Unit	Size	Task	Metric	Dataset Split
TDC.Lipophilicity_AstraZeneca	log-ratio	4,200	Regression	MAE	Scaffold

Leaderboard

Rank	Model	Contact	Link	#Params	MAE ↓
1	Chemprop-RDKit	Kyle Swanson	GitHub , Paper	N/A	0.467 ± 0.006
2	Chemprop	Kyle Swanson	GitHub , Paper	N/A	0.470 ± 0.009
3	BaseBoosting KyQVZ6b2	David Huang	GitHub , Paper	N/A	0.479 ± 0.007
4	MapLight + GNN	Jim Notwell	GitHub , Paper	N/A	0.525 ± 0.003
5	ContextPred	Kexin Huang	GitHub , Paper	2,067,053	0.535 ± 0.012
6	MapLight	Jim Notwell	GitHub , Paper	N/A	0.539 ± 0.002
7	GCN	Kexin Huang	GitHub , Paper	191,810	0.541 ± 0.011
8	AttrMasking	Kexin Huang	GitHub , Paper	2,067,053	0.547 ± 0.024
9	NeuralFP	Kexin Huang	GitHub , Paper	480,193	0.563 ± 0.023
10	AttentiveFP	Kexin Huang	GitHub , Paper	300,806	0.572 ± 0.007
11	RDKit2D + MLP (DeepPurpose)	Kexin Huang	GitHub , Paper	633,409	0.574 ± 0.017
12	Basic ML	Nilavo Boral	GitHub , Paper	N/A	0.617 ± 0.003
13	Euclia ML model	Euclia	GitHub , Paper	50	0.621 ± 0.005
14	CFA	Nan Jiang	GitHub , Paper	N/A	0.626 ± 0.013
15	Morgan + MLP (DeepPurpose)	Kexin Huang	GitHub , Paper	1,477,185	0.701 ± 0.009
16	CNN (DeepPurpose)	Kexin Huang	GitHub , Paper	226,625	0.743 ± 0.020

↓: The lower the better.